

# Temperature-jump induced changes in protein crystals studied with pink beam serial crystallography

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X-ray crystallography experiments typically yield a static average structure of the molecules under investigation. As proteins function as dynamic entities, it is often desirable to obtain additional information about protein dynamics. Uncovering flexible, connected regions helps in understanding protein functions.

A temperature jump (T-jump) allows to thermally activate a molecules by raising its temperature in very short time. In case of protein crystals such a temperature jump can be relatively easy realized with IR laser pulses, which are absorbed by water molecules present in the crystal structure and then lead to a sudden increase of the temperature [1].

We have studied temperature jump induced structural changes in Ribonuclease A crystals with the method of pink beam fixed target serial crystallography [2, 3]. Here the sample is probed with a polychromatic probe pulse arriving at a defined delay after excitation with the IR pump pulse. Due to the high intensity of the polychromatic X-ray pulses it is possible, to perform T-jumps experiments with high temporal resolution down to the nanosecond time scale.

Whereas our data analysis reveals only very small structural changes induced by the temperature jump, we observe systematic and significant time dependent changes of the thermal displacement parameters (B-factors) of the protein molecule.

## References

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- [3] A. Tolstikova et al., IUCRJ, 6(5), 927-937 (2019).